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Taylor series based finite difference approximations of higher-degree derivatives

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Abstract

A new type of Taylor series based finite difference approximations of higher-degree derivatives of a function are presented in closed forms, with their coefficients given by explicit formulas for arbitrary orders. Characteristics and accuracies of presented approximations and already presented central difference higher-degree approximations are investigated by performing example numerical differentiations. It is shown that the presented approximations are more accurate than the central difference approximations, especially for odd degrees. However, for even degrees, central difference approximations become attractive, as the coefficients of the presented approximations of even degrees do not correspond to equispaced input samples.

Keywords: Finite difference approximations; Forward difference approximations; Backward difference approximations; Central difference approximations; Taylor series; Numerical differentiation; Higher-degree derivatives

0. Introduction

Taylor series based finite difference approximations [1–4,6–10] are efficient numerical procedures of approximating the derivatives of a function, at a reference mesh point, by using the values of the function at the neighboring mesh points. Automatic differentiation [5,11] is another efficient and accurate differentiation technique that can be used for the functions, which can be represented by a computer code, but cannot be used for the inputs for which generating functions are not known, as

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is the case in most of the real time applications. In contrast, finite difference approximations do not need to know the generating function of the data, although in some cases this information might be helpful in choosing the best approximation to use. In addition to differentiation, finite difference approximations can be used in finding the numerical solutions of differential and partial differential equations. Some other methods of solving differential and partial differential equations can be found in [12–18].

Depending on the pattern of data samples used to approximate the derivative, Taylor series based finite difference approximations can be divided into three major categories, namely forward, backward and central difference approximations. These approximations use the function values at a set of equally spaced mesh points, to approximate the value of the derivative at the left most, right most and the central mesh points, respectively. The mesh point at which the derivative is approximated is called reference mesh point, and the number of mesh points used in approximation, excluding the reference mesh point defines the order of the approximation.

A finite difference approximation of order N can be obtained by solving N equations obtained directly from Taylor series or by the method of undetermined coefficients [4,6], and gives the derivative at the reference mesh point with an error of the order of $T^N/N!$, where T is the sampling period. Therefore, by increasing the order, generally, the error can be reduced; however, at the same time the complexity involved in obtaining the approximation is drastically increased. Furthermore, the unavailability of relationships to derive the coefficients of an approximation of a certain order, from those of an approximation of a different order, makes it necessary to re-solve a system of linear equations, when there is a need to change the order. Due to these reasons, direct use of these approximations was limited only to smaller orders, and other equivalent forms including those based on interpolating polynomials like Lagrangian, Bessel, Newton-Gregory, Gauss and Sterling interpolating polynomials [1–4,7,10], were used for higher orders. The approximations based on these polynomials can be generated efficiently by using operators [3] and Lozenge diagrams [4]. However, they use difference tables constructed form data samples, and therefore perform the differentiation relatively less efficiently as compared to finite difference approximations, which directly use the data samples.

In [8], we presented closed form expressions for Taylor series based forward, backward and central difference approximations, and presented their coefficients with simple explicit formulas. This makes their determination very simple for any arbitrary order, without any need to solve equations, and there does not remain any need of remembering or recording the coefficients of long approximations or using less efficient equivalent forms. In addition to the first-degree approximations, central difference approximations of higher degrees [1] were also presented in closed forms in [8], and explicit formulas were given for their tap-coefficients, for arbitrary orders.

It was shown in [8], that central difference approximations are more accurate than forward and backward difference approximations, especially for the oscillating and periodic functions. In addition, only central difference approximations have linear phase and can perform differentiation without inducing any nonlinearity in the phase of the differentiated data. However, if the maximum frequency of the differentiated data is close to the Nyquist frequency (half of the sampling frequency), the error

[1] The term 'degree' is used instead of the 'order' of the derivative to avoid the ambiguity with 'order' of the approximation, which is indicator of its length.

for the central difference approximations is also quite high, and in the worst case, relative error can become 100%.

A new type of finite difference approximations was introduced in [9], which use the function values at an even number of mesh points and give the derivative at a reference point lying in the middle of two central mesh points. Like central difference approximations, these new approximations also have linear phase, and do not introduce any nonlinearity in the phase of the differentiated signal. Their computational complexities are also of the same orders as those of central difference approximations and both are equally highly accurate for polynomial inputs. However new approximations are much more accurate for periodic or oscillating functions, especially if the function to be differentiated has high frequency components close to the Nyquist frequency. We presented closed form expressions for these approximations of first-degree derivatives, with the explicit formulas for their coefficients, for an arbitrary order. In this paper, we extend these approximations for derivatives of arbitrary higher degrees and present explicit formulas for their coefficients, for arbitrary orders.

We review the central difference approximations of higher degrees presented in [8] in Section 1, and present the new approximations of higher degrees in Section 2. Accuracy and different characteristics of the two are compared in Section 3 by comparing the results of differentiation of some example functions.

1. Central difference approximations of arbitrary degree

Taylor series based central difference approximation of arbitrary pth degree derivative of a function $f(t)$ at $t = t_0$ can be written for an order $2N$ as [8]

$$f_0^{(p)} = \frac{1}{T^p} \sum_{k=-N}^{N} d_k^{(p)} f_k, \tag{1}$$

where T is the sampling period, f_k denotes the value of function $f(t)$ at $t = t_0 + kT$, and the coefficients $d_k^{(p)}$, which are given for different values of p in Table 1, can be written in a closed form for an arbitrary value of p as

$$d_0^{(p)} = 0 \quad \text{if } p \text{ is odd} \quad \text{otherwise } d_0^{(p)} = -2\sum_{k=1}^{N} d_k^{(p)}, \tag{2}$$

and

$$d_k^{(p)} = (-1)^{k+c_1} \frac{p!}{k^{1+c_2}} C_{N,k} \sum_i \frac{1}{\mathbf{X}(i)^2}, \quad -N \leqslant k \leqslant N, \tag{3}$$

where

$$C_{N,k} = \frac{N!^2}{(N-k)!(N+k)!},$$

c = largest integer less than or equal to $(p-1)/2$,

$c_1 = 1$ if c is even otherwise $c_1 = 0$,

$c_2 = 1$ if p is even otherwise $c_2 = 0$

Table 1
Explicit formulas for tap-coefficients of central difference approximations of arbitrary degree p and arbitrary order $2N$. The factor $C_{N,k}$ stands for $N!^2/(N-k)!(N+k)!$

p	$d_k^{(p)},\ k=\pm1,\pm2,\ldots,\pm N$	$d_0^{(p)}$
1	$(-1)^{k+1}\frac{1}{k}C_{N,k}$	0
2	$(-1)^{k+1}\frac{2!}{k^2}C_{N,k}$	$-2\sum_{k=1}^{N} d_k^{(2)}$
3	$(-1)^{k}\frac{3!}{k}C_{N,k}\sum_{i=1\to N}^{i\neq\lvert k\rvert}\frac{1}{i^2}$	0
4	$(-1)^{k}\frac{4!}{k^2}C_{N,k}\sum_{i=1\to N}^{i\neq\lvert k\rvert}\frac{1}{i^2}$	$-2\sum_{k=1}^{N} d_k^{(4)}$
5	$(-1)^{k+1}\frac{5!}{k}C_{N,k}\sum_{\substack{i=1\to N\\ j=i+1\to N}}^{i,j\neq\lvert k\rvert}\frac{1}{(ij)^2}$	0
6	$(-1)^{k+1}\frac{6!}{k^2}C_{N,k}\sum_{\substack{i=1\to N\\ j=i+1\to N}}^{i,j\neq\lvert k\rvert}\frac{1}{(ij)^2}$	$-2\sum_{k=1}^{N} d_k^{(6)}$
7	$(-1)^{k}\frac{7!}{k}C_{N,k}\sum_{\substack{i=1\to N\\ j=i+1\to N\\ l=j+1\to N}}^{i,j,l\neq\lvert k\rvert}\frac{1}{(ijl)^2}$	0
8	$(-1)^{k}\frac{8!}{k^2}C_{N,k}\sum_{\substack{i=1\to N\\ j=i+1\to N\\ l=j+1\to N}}^{i,j,l\neq\lvert k\rvert}\frac{1}{(ijl)^2}$	$-2\sum_{k=1}^{N} d_k^{(8)}$

and the vector $\mathbf{X}$ of length C_c^{N-1} is generated in the following way:

1. Take a vector $\mathbf{Y}$ containing all integers from 1 to N except k.
2. The vector $\mathbf{X}$ contains the product of all the possible combinations of length c in $\mathbf{Y}$.

For example, for 4th coefficient ($k=4$) in derivative of 5th degree ($p=5$) of order 10 ($N=5$), $\mathbf{Y}=\{1,2,3,5\}$. In this case $c=2$, and $\mathbf{X}=\{\{1\times2\},\{1\times3\},\{1\times5\},\{2\times3\},\{2\times5\},\{3\times5\}\}=\{2,3,5,6,10,15\}$.

2. New finite difference approximations of arbitrary degree

Central difference approximations use the function values at an odd number of mesh points, while the reference point at which derivative is approximated is the central mesh point. In [9] we presented new approximations of first degree, which use the function values at an even number of mesh points and approximate the derivative value at a reference point, which is located in the middle of two central mesh points. In other words, the derivatives of a function $f(t)$ is approximated at a reference mesh point $t = t_0$, by using the function values at the mesh points $t = t_0 + (2k-1)T/2$, where $k = 1, 2, 3, \ldots$. In this section, we extend these approximations to higher degrees.

Taylor series expansion of value of a function $f(t)$ at $t = t_0 + nT$ in terms of the values of the function and its derivatives at $t = t_0$ can be written as

$$f_n = f_0 + (nT)f_0^{(1)} + \frac{(nT)^2}{2!} f_0^{(2)} + \frac{(nT)^3}{3!} f_0^{(3)} + \cdots. \tag{4}$$

For $n = \pm(2k-1)/2$, $k = 1, 2, 3, \ldots, N$, Eq. (4) gives a set of $2N$ equations, each of which can be truncated after $2N+1$ terms to form a system of linear approximate equations, which can be written in matrix form as

$$\mathbf{F} \approx \mathbf{A} \cdot \mathbf{D}, \tag{5}$$

where

$$\mathbf{F} = [f_{1/2} - f_0 \quad f_{-1/2} - f_0 \quad \cdots \quad f_{(2N-1)/2} - f_0 \quad f_{-(2N-1)/2} - f_0]^{\mathrm{T}},$$

$$\mathbf{D} = [f_0^{(1)} \quad f_0^{(2)} \quad f_0^{(3)} \quad \cdots \quad f_0^{(2N)}]^{\mathrm{T}},$$

$$\mathbf{A} = \begin{bmatrix} T/2 & (T/2)^2/2 & \cdots & (T/2)^{2N}/2N! \\ -T/2 & (-T/2)^2/2! & & (-T/2)^{2N}/2N! \\ \vdots & & & \\ (2N-1)T/2 & ((2N-1)T/2)^2/2! & & ((2N-1)T/2)^{2N}/2N! \\ -(2N-1)T/2 & (-(2N-1)T/2)^2/2! & & (-(2N-1)T/2)^{2N}/2N! \end{bmatrix},$$

and the truncated terms in Eq. (4) while obtaining Eq. (5) have negligible magnitude of the order of $T^{2N}/(2N)!$.

Any of the derivatives in $\mathbf{D}$, say pth derivative $f_0^{(p)}$, can be written as the ratio of two determinants $|\mathbf{A}_p|/|\mathbf{A}|$, where the matrix $\mathbf{A}_p$ is obtained by replacing pth column in matrix $\mathbf{A}$ by vector $\mathbf{F}$. Noting that both the matrices $\mathbf{A}_p$ and $\mathbf{A}$ are the same except for the pth column, and have the same power of T in every element of a column, $f_0^{(p)}$ can be written as

$$f_0^{(p)} = \frac{1}{T^p} \frac{|\mathbf{A}_p|_{T=1}}{|\mathbf{A}|_{T=1}}. \tag{6}$$

Calculating the determinant of $\mathbf{A}$ for $T = 1$, for different arbitrary orders $2N$, it is observed that it takes the following closed form:

$$|\mathbf{A}|_{T=1} = \frac{1}{2^{2N}(2N)!!}, \tag{7}$$

where the double factorial of an integer k is defined as $k!! = k(k-2)(k-4)\ldots(\geqslant 1)$. Eq. (6) can now be written as

$$f_0^{(p)} = \frac{2^{2N}(2N)!!}{T^p} |\mathbf{A}_p|_{T=1}. \tag{8}$$

Table 2
Explicit formulas for tap-coefficients of new approximations of arbitrary degree p and arbitrary order $2N$. The factor $C_{N,k}$ stands for $(2N-1)!!^2/(N-k)!(N+k-1)!$

p	$\hat{d}^{(p)}_{(2k-1)/2},\ -N<k\leqslant N$	$\hat{d}^{(p)}_0$
1	$(-1)^{k+1}\dfrac{1}{\left(\frac{2k-1}{2}\right)^2}\hat{C}_{N,k}$	0
2	$(-1)^{k+1}\dfrac{2!}{\left(\frac{2k-1}{2}\right)^3}\hat{C}_{N,k}$	$-2\sum_{k=1}^{N}\hat{d}^{(2)}_{(2k-1)/2}$
3	$(-1)^{k}\dfrac{3!}{\left(\frac{2k-1}{2}\right)^2}\hat{C}_{N,k}\sum_{i=1\to N}^{i\neq\lvert k\rvert}\dfrac{1}{\left(\frac{2i-1}{2}\right)^2}$	0
4	$(-1)^{k}\dfrac{4!}{\left(\frac{2k-1}{2}\right)^3}\hat{C}_{N,k}\sum_{i=1\to N}^{i\neq\lvert k\rvert}\dfrac{1}{\left(\frac{2i-1}{2}\right)^2}$	$-2\sum_{k=1}^{N}\hat{d}^{(4)}_{(2k-1)/2}$
5	$(-1)^{k+1}\dfrac{5!}{\left(\frac{2k-1}{2}\right)^2}\hat{C}_{N,k}\sum_{\substack{i=1\to N\\ j=i+1\to N}}^{i,j\neq\lvert k\rvert}\dfrac{1}{\left(\frac{2i-1}{2}\right)^2\left(\frac{2j-1}{2}\right)^2}$	0
6	$(-1)^{k+1}\dfrac{6!}{\left(\frac{2k-1}{2}\right)^3}\hat{C}_{N,k}\sum_{\substack{i=1\to N\\ j=i+1\to N}}^{i,j\neq\lvert k\rvert}\dfrac{1}{\left(\frac{2i-1}{2}\right)^2\left(\frac{2j-1}{2}\right)^2}$	$-2\sum_{k=1}^{N}\hat{d}^{(6)}_{(2k-1)/2}$
7	$(-1)^{k}\dfrac{7!}{\left(\frac{2k-1}{2}\right)^2}\hat{C}_{N,k}\sum_{\substack{i=1\to N\\ j=i+1\to N\\ l=j+1\to N}}^{i,j,l\neq\lvert k\rvert}\dfrac{1}{\left(\frac{2i-1}{2}\right)^2\left(\frac{2j-1}{2}\right)^2\left(\frac{2l-1}{2}\right)^2}$	0
8	$(-1)^{k}\dfrac{8!}{\left(\frac{2k-1}{2}\right)^3}\hat{C}_{N,k}\sum_{\substack{i=1\to N\\ j=i+1\to N\\ l=j+1\to N}}^{i,j,l\neq\lvert k\rvert}\dfrac{1}{\left(\frac{2i-1}{2}\right)^2\left(\frac{2j-1}{2}\right)^2\left(\frac{2l-1}{2}\right)^2}$	$-2\sum_{k=1}^{N}\hat{d}^{(8)}_{(2k-1)/2}$

We simplified Eq. (8) and obtained the formulas of derivatives for different values of p and a large set of different values of N, and found that, for arbitrary values of p and N, they can be written in a closed form as

$$f^{(p)}_0 = \frac{1}{T^p}\left(\hat{d}_0 f_0 + \sum_{k=-N+1}^{N}\hat{d}^{(p)}_{(2k-1)/2} f_{(2k-1)/2}\right) \tag{9}$$

where the explicit formulas for the coefficients $\hat{d}$ are listed in Table 2 for different values of p, and can be written in closed form for arbitrary values of p and N as

$$\hat{d}^{(p)}_{(2k-1)/2} = (-1)^{k+c_1}\frac{p!}{((2k-1)/2)^{2+c_2}}\hat{C}_{N,k}\sum_i \frac{1}{\hat{\mathbf{X}}(i)^2}, \quad -N<k\leqslant N,$$

$$\hat{d}_0^{(p)} = -2 \sum_{k=-N+1}^{N} \hat{d}^{p}_{(2k-1)/2}, \tag{10}$$

where

$$\hat{C}_{N,k} = \frac{(2N-1)!!^2}{2^{2N}(N-k)!(N+k-1)!}$$

and the vector $\hat{\mathbf{X}}$ is generated in the following way:

1. Take a vector $\hat{\mathbf{Y}}$ containing the values $(2i-1)/2$ for $i = 1, 2, \ldots, N$ and $i \neq k$.
2. Generate $\hat{\mathbf{X}}$ from $\hat{\mathbf{Y}}$ in the exactly the same way as $\mathbf{X}$ was generated from $\mathbf{Y}$ in Eq. (3). For example, for 4th coefficient ($k = 4$) in derivative of 5th degree ($p = 5$) of order 10 ($N = 5$), $\hat{\mathbf{Y}} = \{1/2, 3/2, 5/2, 9/2\}$ and $\hat{\mathbf{X}} = \{3/4, 5/4, 9/4, 15/4, 27/4, 45/4\}$.

It can be noted from Eqs. (1) and (9) that the computational complexities involved in using central difference and new approximations are of the same order.

3. Discussion

By looking at Tables 1 and 2, different patterns of coefficients can be observed for approximations of even and odd degrees, both for central difference and new approximations presented in the previous section. Approximations of even degrees have even-symmetric coefficients while approximations of odd degrees have odd-symmetric coefficients, and this affects their characteristics, separating them into two different classes.

To observe the characteristics of the approximations of even and odd degrees, we have listed the errors in second-degree and third-degree differentiation of some example functions, in Tables 3 and 4, respectively, using both central difference and the new approximations. Two different sampling periods and orders are used in each table. The columns headed by N and C show the errors by using new formulas and central difference approximations, respectively. To minimize the round off error, calculations are carried out with a precision of 100 decimal points. Except in the first two rows for polynomials, for which relative errors become indeterminate, all the entries in the table give percentage relative errors. While observing that new approximations are more accurate than central difference approximations, for any type of input, certain important points can be noted as given below:

1. Both central difference and new approximations are highly accurate for polynomial functions. An approximation of order $2N$ is exact for a polynomial t^k, where $k \leqslant 2N$ for approximations of odd degrees, and $k \leqslant 2N+1$ for approximations of even degrees. This can be understood by looking at the terms truncated in Eq. (4) while obtaining Eq. (5). These terms have derivatives of minimum degree $2N+1$ and therefore become zero for a polynomial t^k, $k \leqslant 2N$. For approximations of even degrees, the first truncated terms of Eq. (4) are cancelled out due to even-symmetric coefficients and minimum degree of derivatives in error terms is $2N+2$.
2. All approximations are very accurate for periodic and oscillating functions as well, when the maximum frequency of the function is well below the Nyquist frequency. The error is increased,

Table 3
Errors in second-degree numerical differentiation of example functions with central difference and new approximations of two different orders and sampling periods

Function	Order = 6				Order = 10			
	$T=10^{-3}$		$T=10^{-6}$		$T=10^{-3}$		$T=10^{-6}$	
	N	C	N	C	N	C	N	C
$t-t^7$	0	0	0	0	0	0	0	0
t^8	7E-18	7.2E-17	7E-36	7.2E-35	0	0	0	0
$e^{-\pi t}$	1.7E-17	1.7E-16	1.7E-35	1.7E-34	3.4E-29	5.6E-28	3.4E-59	5.6E-58
$e^{-100\pi t}$	1.7E-5	1.7E-4	1.7E-23	1.7E-22	3.5E-9	5.8E-8	3.4E-39	5.6E-38
$\cos(\pi t)$	1.7E-17	1.7E-16	1.7E-35	1.7E-34	3.4E-29	5.6E-28	3.4E-59	5.6E-58
$\cos(100\pi t)$	1.7E-5	1.7E-4	1.7E-23	1.7E-22	3.3E-9	5.5E-8	3.4E-39	5.6E-38
$\cos(500\pi t)$	0.207	1.831	2.6E-19	2.7E-18	0.02	0.26	3.3E-32	5.5E-31
$\cos(100\pi t)+\cos(500\pi t)$	0.198	1.761	2.5E-19	2.6E-18	0.018	0.251	3.2E-32	5.3E-31
$\cos(1000\pi t)$	6.694	38.76	1.7E-17	1.7E-16	4.04	30.83	3.4E-29	5.6E-28

Table 4
Errors in third-degree numerical differentiation of example functions with central difference and new approximations of two different orders and sampling periods

Function	Order = 6				Order = 10			
	$T=10^{-3}$		$T=10^{-6}$		$T=10^{-3}$		$T=10^{-6}$	
	N	C	N	C	N	C	N	C
$t-t^6$	0	0	0	0	0	0	0	0
t^7	9.7E-11	2.9E-10	9.7E-23	2.9E-22	0	0	0	0
$e^{-\pi t}$	1.9E-10	5.7E-10	1.9E-22	5.7E-22	5.9E-22	3E-21	5.9E-46	3E-45
$e^{-100\pi t}$	0.019	0.058	1.9E-14	5.7E-14	6E-6	3.1E-5	5.9E-30	3E-29
$\sin(\pi t)$	1.9E-10	5.7E-10	1.9E-22	5.7E-22	5.9E-22	3E-21	5.9E-46	3E-45
$\sin(100\pi t)$	0.019	0.056	1.9E-14	5.7E-14	5.7E-6	2.9E-5	5.9E-30	3E-29
$\sin(500\pi t)$	8.779	22.6	1.2E-11	3.6E-11	1.205	4.959	2.3E-24	1.2E-23
$\sin(100\pi t)+\sin(500\pi t)$	8.709	22.41	1.2E-11	3.5E-11	1.196	4.919	2.3E-24	1.2E-23
$\sin(1000\pi t)$	61.3	100	1.9E-10	5.7E-10	47.83	100	5.9E-22	3E-21

if the maximum frequency of the input function is increased, and the worst case is observed at the Nyquist frequency. In such situation, error in central difference approximations of odd degrees of any order increases to 100% (see last row of Table 4). Other approximations also have large errors at the Nyquist frequency, however their errors can be reduced by increasing their orders.

3. Reducing the sampling period reduces the error. This in fact means increasing the sampling frequency and therefore reducing the ratio of the maximum frequency to the Nyquist frequency. It can also be noted (see second last rows) that if the input has more than one frequency components of same amplitude, the relative error is slightly less but of the order of that caused due to the single highest frequency.

From the above results, and the patterns of coefficients of approximations in Tables 1 and 2, we get important information of applications of different approximations as given below:

1. It can be seen from Table 2 that for even values of p, the coefficient $\hat{d}_0^{(p)}$ is not zero, and hence the obtained set of coefficients does not correspond to equally spaced samples. This means that new approximations of even degrees cannot be used to differentiate the equispaced samples of data, for which the generating function is not known. However, they can be used for solving differential and partial differential equations or numerical differentiation of known functions, for which value can be obtained at any mesh point. On the other hand, central difference approximations given by Table 1, do not have such restriction and can be used for equispaced input data, whether its input function is known or not.
2. For odd values of p, the value of $\hat{d}_0^{(p)}$ is always zero, and can be ignored for new approximations to get set of coefficients $\hat{d}_{(2k-1)/2}^{(p)}$ corresponding to equally spaced samples of data. Therefore, both central difference and new approximations of odd degrees can be used for solution of differential and partial differential equations, as well as for numerical differentiation of equispaced data, whether its generating function is known or not.

4. Conclusions

Central difference and a new type of finite difference approximations of higher-degree derivatives of a function have been presented in closed forms. These approximations can be used for numerical differentiation and solution of differential and partial differential equations. Explicit formulas are presented for their coefficients, which make their determination very easy for arbitrary values of order and degree.

Unlike those of general finite different approximations, coefficients of new approximations of even degrees do not correspond to equispaced mesh points and therefore they can be used for numerical differentiation of known functions only. For even-degree derivatives of equispaced data, for which generating function is not known, central difference approximations can be used, which compared to new approximations, have a slightly lower but comparable accuracy.

All the approximations are highly accurate for low frequency input functions, and their performance deteriorates at higher frequencies. Especially the error in central difference approximations of odd degrees increases to 100% at the Nyquist frequency. Therefore, for odd degree derivatives, new approximations can be preferred over central difference approximations for all the applications.

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